Composite fermion theory of correlated electrons in semiconductor quantum dots in high magnetic fields

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Interacting electrons in a semiconductor quantum dot at strong magnetic fields exhibit a rich set of states, including correlated quantum fluids and crystallites of various symmetries. We develop in this paper a perturbative scheme based on the correlated basis functions of the composite-fermion theory, that allows a systematic improvement of the wave functions and the energies for low-lying eigenstates. For a test of the method, we study systems for which exact results are known, and find that practically exact answers are obtained for the ground state wave function, ground state energy, excitation gap, and the pair correlation function. We show how the perturbative scheme helps resolve the subtle physics of competing orders in certain anomalous cases.

There is a strong motivation for developing theoretical tools for obtaining a precise quantitative description of interacting electrons in confined geometries, for example in a semiconductor quantum dot, because of their possible relevance to future technology [1]. Exact diagonalization is possible in some limits but restricted to very small numbers of electrons, and does not give insight into the underlying physics. For larger systems, one must necessarily appeal to approximate methods. The standard Hartree-Fock or density functional type methods provide useful insight, but are often not very accurate for these strongly correlated systems. The aim of this paper is to demonstrate that a practically exact quantitative description is possible for a model quantum dot system, facilitated by the ability to construct low-energy correlated basis functions.

Our concern will be with the solution of

$$H = \sum_j \frac{1}{2m_b}\left(\boldsymbol{p}_j + \frac{e}{c}\boldsymbol{A}_j\right)^2 + \sum_j \frac{m_b}{2}\omega_0^2 r_j^2 + \sum_{j<k} \frac{e^2}{\epsilon r_{jk}} \quad (1)$$

which contains N interacting electrons in two dimensions, confined by a parabolic potential and subjected to a magnetic field. The parameter m_b is the band mass of the electron, ω_0 is a measure of the strength of the confinement, ϵ is the dielectric constant of the host semiconductor, and $r_{jk} = |\boldsymbol{r}_j - \boldsymbol{r}_k|$. We will consider the limit of a large magnetic field ($\omega_c = eB/m_bc \gg \omega_0$), when it is a good approximation to take electrons to be confined to the lowest Landau level (LL). In that limit, the energy eigenvalues have the form $E(L) = E_c(L) + V(L)$ where the contribution from the confinement potential is explicitly known as a function of the total angular momentum L: $E_c(L) = (\hbar/2)[\Omega - \omega_c]L$, with $\Omega^2 = \omega_c^2 + 4\omega_0^2$, and $V(L)$ is the interaction energy of electrons without confinement, but with the magnetic length replaced by an effective magnetic length given by $\ell \equiv \sqrt{\hbar/m_b\Omega}$. Thus, the problem is reduced to finding the interaction energy V (which will be quoted below in units of $e^2/\epsilon\ell$) as a function of the angular momentum L. Exact results, known

for a range of N and L values from a numerical diagonalization of the Hamiltonian, provide a rigorous and unbiased benchmark for any theoretical approach. Exact studies have shown [2] a correlated liquid like state at small L, but a crystallite at relatively large L, as may be expected from the fact that the system becomes more and more classical as L increases. (The ground state in the classical limit is a crystal [3].) Hartree-Fock studies have been performed for the quantum crystallite [4, 5].

We will apply the composite fermion (CF) theory [6] to quantum dot states [7, 8, 9]. The central idea is a mapping between strongly interacting electrons at angular momentum L and weakly interacting electrons at $L^* \equiv L - pN(N-1)$. In particular, a correlated basis $\{\Psi_\alpha^L\}$ for the low energy states of interacting electrons at L can be constructed from the trivial, orthonormal Slater determinant basis for non-interacting electrons at L^*, denoted by $\{\Phi_\alpha^{L^*}\}$, in the following manner:

$$\Psi_\alpha^L = \mathcal{P}\prod_{j<k}(z_j - z_k)^{2p}\Phi_\alpha^{L^*} . \quad (2)$$

Here, $z_j = x_j - iy_j$ denotes the position of the jth electron, $2p$ is the vorticity of composite fermions, and $\mathcal{P}$ indicates projection into the lowest LL. (Electrons at L^* in general occupy several Landau levels.) The symbol $\alpha = 1, 2, \cdots, D^*$ labels the D^* Slater determinants included in the study. In general, the basis $\{\Psi_\alpha^L\}$ is not linearly independent, so its dimension, D_{CF}, may not be equal to D^* ($D_{CF} \leq D^*$). The advantage of working with the correlated CF basis is that D_{CF} is drastically smaller than D_{ex}, the dimension of the lowest LL Fock space at L (which is also the dimension of the matrix that must be diagonalized for obtaining exact results). Fig. (1) illustrates some basis functions at $L = 95$.

At a back-of-the-envelope level, one can compare the exact interaction energy at L to the kinetic energy of *free* fermions at L^*, with the cyclotron energy treated as an adjustable parameter [7]. That reproduces the qualitative behavior for the L dependence of the exact energy
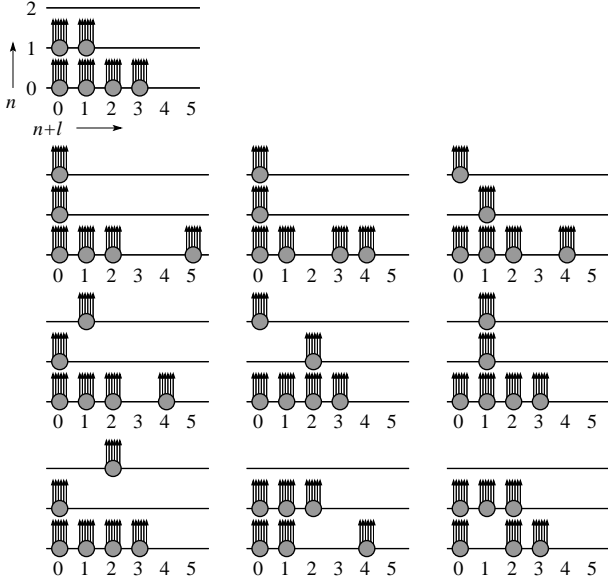
FIG. 1: Schematic depiction of Slater determinant basis states for $N = 6$ electrons at $L = 95$, which maps into $L^* = 5$ with $2p = 6$. The single electron orbitals at $L^* = 5$ are labeled by two quantum numbers, the LL index $n = 0, 1, ...,$ and the angular momentum $l = -n, -n+1, ...$ The x-axis labels $n+l$ and the y-axis n. The dots show the occupied orbitals forming the Slater determinants $\Phi_\alpha^{L^*=5}$ relevant up to the first order. The state shown at the top left has the lowest kinetic energy (if the kinetic energy is measured relative to the lowest Landau level, then, in units of the cyclotron energy, the total kinetic energy of this state is two). The other nine states have one higher unit of kinetic energy. The basis states $\Psi_\alpha^{L=95}$ are obtained according to Eq. (2), through multiplication by $\prod_{j<k}(z_j - z_k)^6$, which converts electrons into composite fermions carrying six vortices. That is shown schematically by six arrows on each dot. The single state at the top is relevant at the zeroth order, and all ten basis states are employed at the first order. (In fact, there are a total of 12 linearly independent states $\Phi_\alpha^{L^*}$ at the first order for $L^* = 5$, but they produce only ten linearly independent states Ψ_α^L at $L = 95$.)

L	V_{ex}	$V_{\mathrm{CF}}^{(0)}$	$V_{\mathrm{CF}}^{(1)}$	D_{ex}	$D_{\mathrm{CF}}^{(0)}$	$D_{\mathrm{CF}}^{(1)}$
79	2.1570	2.1610(2)	2.1573(3)	26207	4	55
80	2.1304	2.1332(1)	2.1307(1)	28009	2	33
81	2.1286	2.1302(1)	2.1289(2)	29941	1	20
82	2.1226	2.1261(4)	2.1229(5)	31943	10	86
83	2.1090	2.1141(7)	2.1093(2)	34085	5	50
84	2.0893	2.0941(1)	2.0903(2)	36308	2	26
85	2.0651	2.0692(1)	2.0655(1)	38677	1	13
86	2.0651	2.0694(5)	2.0656(2)	41134	5	48
87	2.0543	2.0552(2)	2.0546(2)	43752	2	24
88	2.0462	2.0496(1)	2.0466(2)	46461	9	58
89	2.0279	2.0330(3)	2.0290(3)	49342	3	27
90	2.0054	2.0097(1)	2.0064(1)	52327	1	9
91	2.0054	2.0098(3)	2.0065(2)	55491	3	25
92	1.9989	2.0013(1)	1.9996(2)	58767	8	48
93	1.9852	1.9861(1)	1.9851(3)	62239	2	20
94	1.9715	1.9764(2)	1.9726(2)	65827	4	36
95	1.9506	1.9549(2)	1.9516(2)	69624	1	10
96	1.9506	1.9551(2)	1.9516(4)	73551	2	18
97	1.9447	1.9484(1)	1.9456(5)	77695	5	32
98	1.9347	1.9381(3)	1.9359(4)	81979	9	49
99	1.9189	1.9228(1)	1.9217(4)	86499	1	17
100	1.9001	1.9034(2)	1.9014(3)	91164	2	26
101	1.9001	1.9033(2)	1.9014(1)	96079	4	41
102	1.8947	1.8977(2)	1.8959(3)	101155	7	58
103	1.8855	1.8880(2)	1.8863(2)	106491	12	83
104	1.8712	1.8736(2)	1.8729(1)	111999	18	111
105	1.8533	1.8617(2)	1.8542(3)	117788	1	28
106	1.8533	1.8618(1)	1.8538(4)	123755	1	39
107	1.8483	1.8555(2)	1.8488(4)	130019	2	55
108	1.8396	1.8463(2)	1.8402(4)	136479	3	74

TABLE I: Exact ground state energy (V_{ex}) and the ground state energy obtained from the zeroth ($V_{\mathrm{CF}}^{(0)}$) and the first-order ($V_{\mathrm{CF}}^{(1)}$) CF theory for $N = 6$. The dimensions of the bases diagonalized are D_{ex}, $D_{\mathrm{CF}}^{(0)}$ and $D_{\mathrm{CF}}^{(1)}$, respectively. The statistical uncertainty arising from Monte Carlo sampling is given in parentheses.

for small L [7], but discrepancies are known to appear at larger L [2, 5].

For a more substantive test of the theory, it is necessary to obtain the energy spectrum by diagonalizing the Hamiltonian of Eq. 1 in the correlated basis functions of Eq. (2). The CF-quasi-Landau level mixing is treated as a small parameter, and completely suppressed at the simplest approximation, which we refer to as the zeroth order approximation. Here, the correlated basis states at L are obtained by restricting the basis $\{\Phi_\alpha\}$ to all states with the lowest kinetic energy at L^* (with p always chosen so as to give the smallest dimension).

Diagonalization in the correlated CF basis is technically involved, but efficient methods for generating the basis functions as well as all of the matrix elements required for Gram-Schmidt orthogonalization and diagonalization have been developed using Metropolis Monte

Carlo sampling. We refer the reader to earlier literature for full details [8, 10].

A diagonalization of the Hamiltonian in the zeroth level basis produces energies and wave functions for $D_{\mathrm{CF}}^{(0)}$ low-lying states. The interaction energy and the wave function for the ground state will be denoted $V_{CF}^{(0)}$ and $\Psi_{CF}^{(0)}$, respectively. We have carried out [11] extensive calculations for a large range of L for up to ten particles, and found that the CF theory reproduces the qualitative behavior of the energy as a function of L all the way to the largest L for which exact results are known. We show in Table I results for $N = 6$ electrons in the angular momentum range $79 \leq L \leq 108$, which spans both liquid and crystal-like ground states. Ref. [11] shows a comparison of the exact pair correlation function with that calculated from $\Psi_{CF}^{(0)}$ for $L = 95$ (where there is a unique CF wave function); surprisingly, the CF theory, originally intended for the liquid state, au-

L	$\mathcal{O}^{(0)}$	$\mathcal{O}^{(1)}$	L	$\mathcal{O}^{(0)}$	$\mathcal{O}^{(1)}$
95	0.902	0.988	102	0.927	0.985
96	0.892	0.988	103	0.943	0.978
97	0.898	0.989	104	0.946	0.972
98	0.908	0.985	105	0.714	0.989
99	0.767	0.859	106	0.710	0.987
100	0.936	0.982	107	0.735	0.988
101	0.936	0.981	108	0.781	0.990

TABLE II: Overlaps between exact ground states and CF ground states obtained at the zeroth ($\mathcal{O}^{(0)}$) and the first order($\mathcal{O}^{(1)}$). The statistical uncertainty from Monte Carlo sampling does not affect the first three significant figures.

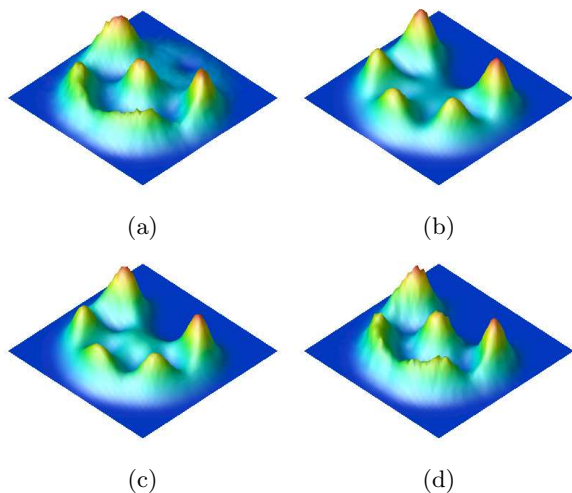(a)   (b)

(c)   (d)

FIG. 2: Pair correlation function for $N = 6$ electrons at $L = 99$. The position of one particle is fixed on the outer ring, coincident with the position of the missing peak. The ground state wave function used in the calculation is obtained from (a) exact diagonalization; (b) the zeroth-order CF theory; (c) the first-order CF theory; (d) the second-order CF theory. The "noise" in (a) and (d) results from the relatively large statistical uncertainty in Monte Carlo because of the more complicated wave function.

tomatically produces also a crystallite at large L, even though no crystal structure has been put into the theory by hand [12]. Table II gives the overlaps defined as:
$$\mathcal{O}^{(0)} \equiv |\langle \Psi_{\mathrm{CF}}^{(0)}|\Psi_{\mathrm{ex}}\rangle| / \sqrt{\langle \Psi_{\mathrm{CF}}^{(0)}|\Psi_{\mathrm{CF}}^{(0)}\rangle\langle \Psi_{\mathrm{ex}}|\Psi_{\mathrm{ex}}\rangle}.$$

While the zeroth level description is quite good, the following deviations from the exact solution may be noted. (i) The overlaps are in the range 0.70-0.94, which are not as high as the overlaps ($\sim$0.99) for incompressible ground states in the spherical geometry. (ii) The energies are within 0.5% of the exact ones, which is quite good but could be further improved. (iii) In the crystallite, the particles are somewhat less strongly localized in the CF wave function than in the exact ground state. See Ref. [11]. (iv) The symmetry of the crystallite is pre-

dicted correctly with the exception of $L = 99$, where the CF theory predicts a $(0, 6)$ crystallite [Fig. 2(b)], that is, with all six particles on an outer ring, whereas the exact solution shows a $(1, 5)$ crystallite [Fig. 2(a)], which has five particles on the outer ring and one at the center. (v) A successful theory must explain not only the ground state but also excited states, especially the low-energy ones. We have considered the gap between the two lowest eigenstates. The zeroth-order theory does not give, overall, a satisfactory account of it. In some instances (e.g., $L = 81, 85, 90, 95, 99, 105, 106$ for $N = 6$), the CF theory gives no information on the gap, because the basis contains only a single state here ($D_{CF}^{(0)} = 1$); in many other cases, the gap predicted by the CF theory is off by a factor of two to three.

These discrepancies have motivated us to incorporate CF-quasi-LL mixing perturbatively. (We stress that CF-quasi-LL mixing implies LL mixing at L^*, but the basis states at L are, by construction, always within the lowest LL.) At the first order, we include basis states Φ^{L^*} at L^* with one more unit of the kinetic energy, which produces a larger basis at L through Eq. (2). The basic idea is illustrated for the case of $N = 6$ and $L = 95$ ($L^* = 5$, $2p = 6$) in Fig. 1.

In a similar way we have constructed correlated basis functions at each angular momentum in the range $79 \leq L \leq 108$. As shown in Table I $D_{\mathrm{CF}}^{(1)}$, the dimension of the basis in the first-order theory is larger than $D_{\mathrm{CF}}^{(0)}$ but still far smaller than D_{ex}. A diagonalization of the Hamiltonian in this basis produces the ground state energy $V_{CF}^{(1)}$ and ground state wave function $\Psi_{CF}^{(1)}$. Leaving aside $L = 99$, which we shall discuss separately, the following observations can be made: (i) The energies are essentially exact. As shown in Table I, the deviation from the exact energy is reduced to <0.1%, in fact, to <0.05% in most cases. (ii) The overlaps from the first-order theory, $\mathcal{O}^{(1)} \equiv |\langle \Psi_{\mathrm{CF}}^{(1)}|\Psi_{\mathrm{ex}}\rangle| / \sqrt{\langle \Psi_{\mathrm{CF}}^{(1)}|\Psi_{\mathrm{CF}}^{(1)}\rangle\langle \Psi_{\mathrm{ex}}|\Psi_{\mathrm{ex}}\rangle}$, are given in Table II. They are uniformly excellent (0.98-0.99) in the entire L range studied. (iii) The improvement by the first order perturbation theory is also man-
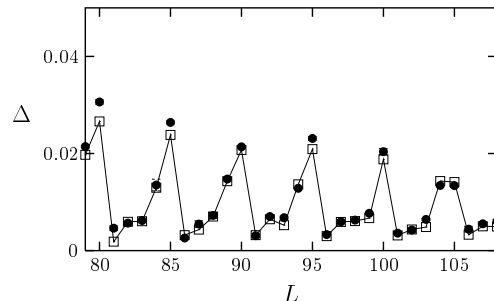

FIG. 3: Comparison of the exact excitation gaps ($\square$) for $N = 6$ with the gaps obtained in the first-order CF theory ($\bullet$).

L	D_{ex}	$D_{CF}^{(2)}$	V_{ex}	$V_{CF}^{(2)}$	$\mathcal{O}^{(2)}$
99	86499	76	1.9189	1.9193(3)	0.995

TABLE III: Comparison of the second order CF theory with exact results for the $L = 99$ ground state. $D^{(2)}$ is the dimension of the correlated CF basis, $V_{CF}^{(2)}$ is the CF prediction for the ground state energy, and $\mathcal{O}^{(2)}$ is the overlap between the CF and the exact wave functions.

ifest in the pair-correlation functions, which are now indistinguishable from the exact ones at arbitrary L. That is not surprising, given the high overlaps. (iv) As seen in Fig. 3 the first-order theory reproduces the qualitative behavior of the excitation gap as a function of L, and also gives very good quantitative values. The maximum gaps are correlated with the states where a downward cusp appears in the plot of $V(L)$, consistent with the higher stability of these ground states.

Finally, we discuss the case of $L = 99$. Here, the zeroth order CF theory predicts a wrong symmetry for the crystallite [Fig. 2(b)]. As seen in Fig. 2(c), the first order correction also fails to recover the correct symmetry. That is also reflected in the fact that the modified ground state of the first-order theory yields a relatively small overlap of ~ 0.86, and the energy is off by a relatively large 0.15%. A closer inspection of the correlations in Fig. 2(c) reveals a slight broadening of the hexagonal structure in the outer-ring, combined with an appearance of a small mound at the center, suggesting that the structure here may be a superposition of (0,6) and (1,5) crystallites. This has motivated us to incorporate the next (second) order corrections. The basis dimension $D_{CF}^{(2)}$ is now further enlarged, but Monte Carlo still produces reliable results. The CF ground state wave function obtained at this level is extremely accurate: the pair correlation function shown in Fig. 2(d) compares well to the exact one, and, as seen in Table III, the energy and the overlaps are close to perfect. The origin of the difficulty can be understood from the fact that the (0,6) and the (1,5) crystallites are nearly degenerate in the classical limit [3], making them both competitive.

We have focused in this work on cases where the exact results are known, because the aim was to test the applicability of the CF theory to quantum dots. The theory can be extended to much larger systems, where exact diagonalization is not possible; in such cases, one would need to increase the accuracy perturbatively until sufficient convergence is achieved. The method developed here should also prove useful for multiple coupled quantum dots [13] and rapidly rotating atomic Bose-Einstein condensates [14].

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